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Positronium formation for hydrogen using Schwinger's principle for rearrangement collisions

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Abstract Positronium formation in positron-hydrogen collisions is studied using Schwinger's principle for rearrangement collisions in the momentum space at low energies of positron impact in the range 6.8–15.0 eV. Only eight terms in a correlated basis expansion in both the direct and rearrangement channels are required to predict accurate cross sections for S-, P-, D-, and higher partial waves upto L=15 in agreement with the Kohn-Hulthén variational results available in the literature. Our findings indicate that there exist critical angles due to destructive interference between partial-wave contributions to the scattering amplitude. These are displayed through surface plots of the differential cross-section. The predicted total cross sections are in accord with the observed data of the Wayne State experiment [*Phys. Rev.* **A55** 361 (1997)]

Keywords Positronium, Schwinger's principle, rearrangement collisions

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1. Introduction

The Schwinger variational principle has been utilised in the momentum space in recent years to study positron hydrogen collisions using a discrete correlated basis set [1]. Accurate results to the elastic scattering have been reported for S-, P-, D-, and higher partial waves upto $L=12$ by this method in the incident positron energy-range 0.136 – 30.6 eV. The method has been extended to study the rearrangement collision process of positronium formation in positron-hydrogen collisions for the S-wave only with reasonable success [2].

In this work, following Joachain [3], we have formulated the Schwinger variational principle appropriate for rearrangement collisions in the momentum space. Instead of the K-matrix, we have analyzed the rearrangement scattering amplitude in a discrete basis set expansion and have applied it to positronium formation in positron-hydrogen collisions at low energies in the energy-range 6.8 – 15.0 eV. It is possible for us to obtain accurate values of the positronium formation cross section in this energy range with only eight terms in the basis expansion. The results are compared with the theoretical and experimental data available in the literature [4-9].

2. Theory

Following Joachain [3], we are able to write the 'prior' form of the scattering amplitude for rearrangement collisions using Schwinger's principle in a perfect three-body scattering system : $1 + (2,3) \rightarrow (1,2) + 3$ as

$$\left[T_{fi}(\beta k_f, \alpha k_i)\right] = <\Phi_f \; V_i + (V_f - V_i)G_i^+ V_i \; \Psi_i^+ > + <\Psi_f^- \; V \; \Phi_i >$$

$$- <\Psi_f^- \; V - VG^+V \left|\Psi^+\right. > \tag{1}$$

in which Φ_i, Φ_f denote respectively the plane-wave states in the direct and positronium formation channels, V_i, V_f are the corresponding residual interactions with the full Hamiltonian of the system given by $H = H_i + V_i = H_f + V_f$ such that the channel states satisfy $H_i\Phi_i = E_i\Phi_i$, $H_f\Phi_f = E_f\Phi_f$, whereas the Green's operator $G_i^+ = 1/(E - H_i + i\varepsilon)$. We expand Ψ_i^+ and Ψ_f^- into discrete basis sets of single channel functions :

$$\Psi_i^+ = \sum a_m u_m, \quad \Psi_f^- = \sum b_n v_n, \tag{2}$$

where $a_m = \left(a_m^{(1)}, a_m^{(2)}\right)$, $b_n = \left(b_n^{(1)}, b_n^{(2)}\right)$ are linear constants.

It is useful now to define "two-body" scattering amplitudes in terms of these basis functions .

$$A_{fm}(\beta k_f, \alpha k_i) = \left(-\mu_f / 2\pi\right) < \Phi_f | V_i + V_d^+ G_i^+ V_i | u_m > \quad (V_d^+ = V_f - V_i) \tag{3}$$

$$A_{ni}(\beta k_f, \alpha k_i) = \left(-\mu_f / 2\pi\right) < v_n \left| V_i \right| \Phi_i >, \tag{4}$$

$$A_{nm}(\beta k_f, \alpha k_i) = \left(-\mu_f / 2\pi\right) < v_n \left| V_i \right| u_m >, \tag{5}$$

and the double-scattering amplitude

$$D_{nm}(\beta k_f, \alpha k_i) = A_{nm}(\beta k_f, \alpha k_i)$$

$$- \frac{i}{(2\pi)^3} \sum_\gamma \left(-\frac{2\pi}{\mu_\gamma} \right) \int dk'' \frac{A_{n\gamma}(\beta k_f, \gamma k'') \, A_{\gamma m}(\gamma k'', \gamma k_i)}{E - E_\gamma'' + i\varepsilon} \tag{6}$$

where $A_{n\gamma}(\beta k_f, \gamma k_i'')$, $A_{\gamma m}(\gamma k'', \alpha k_i)$ are defined for the intermediate plane-wave states $|\Phi_\gamma''$ belonging to the channel γ of the Hamiltonian H_i, and the three-body amplitude as

$$\left[A_{fi}(\beta k_f, \alpha k_i)\right] = \left(-\mu_f / 2\pi\right)\left[T_{fi}(\beta k_f, \alpha k_i)\right] \tag{7}$$

with the final channel reduced mass $\mu_f = (m_1 + m_2)\, m_3 / ((m_1 + m_2) + m_3)$, and the reduced mass in channel γ, $\mu_\gamma = m_1\,(m_2 + m_3) / (m_1 + (m_2 + m_3))$.

We now perform the partial-wave analysis in the usual way and optimise the linear variational constants a_m, b_n, using the stationary character of $\left[A_{fi}^{(L)}(\beta k_f, \alpha k_i)\right]$:

$$\frac{\partial}{\partial a^{(p)}}\left[A_{fi}^{(L)}\right]=0=\frac{\partial}{\partial b^{(q)}}\left[A_{fi}^{(L)}\right], \quad p,q=1,2,\ m,n=1,2,\ldots,N, \tag{8}$$

to obtain finally the stationary expression of the Schwinger variational scattering amplitude for positronium formation in positron-hydrogen collisions for the partial-wave L as :

$$\left[A_{fi}^{(L)}(\beta k_f,\alpha k_i)\right]=\sum_{m,n}\sum_{p,q}A_{fm}^{(L)(fp)}(\beta k_f,\alpha k_i)\,D_{nm}^{(L)(pq)^{-1}}\,A_{ni}^{(L)(qi)}(\beta k_f,\alpha k_i) \tag{9}$$

where the 'input' two-body partial-wave amplitudes are all given in terms of the basis functions u_m, v_n in the direct and rearrangement channels, respectively, which are chosen in the forms :

$$u_m(\mathbf{r}_1,\mathbf{r}_2)=\Phi_i(\mathbf{r}_1,\mathbf{r}_2)\,\xi_m(\mathbf{r}_1,\mathbf{r}_2) \tag{10}$$

$$v_n(\mathbf{r}_1,\mathbf{r}_2)=\Phi_f(\mathbf{r}_{12},\mathbf{s}_{12})\,\xi_n(\mathbf{r}_1,\mathbf{r}_2) \tag{11}$$

with the channel plane-wave states

$$\Phi_i(\mathbf{r}_1,\mathbf{r}_2)=exp(i\mathbf{k}_i.\mathbf{r}_1)\,\phi_i(\mathbf{r}_2) \tag{12}$$

$$\Phi_f(\mathbf{r}_{12},\mathbf{s}_{12})=exp(i\mathbf{k}_f.\mathbf{s}_{12})\,\eta_f(\mathbf{r}_{12}) \tag{13}$$

and the same correlation function for both the direct and rearrangement channels .

$$\xi_m(\mathbf{r}_1,\mathbf{r}_2)=(-1)^{m-1}e^{-\alpha_m r_1}/(b\,r_{12}+a)^{m_0-1}, \tag{14}$$

s.t. $\alpha_{2m-1}=0$, $\alpha_{2m}=p$; $m_0=1$ for $m=1,2$; $m_0=2$ for $m=3,4$; $m_0=3$ for $m=5,6$; $m_0=4$ for $m=7,8$, *etc*. In fact, we have taken $b=1.0$ and varied the non-linear variational parameters a and p to make the Schwinger variational amplitude (9) stationary.

3. Results and discussion

The correlation functions (14) are found to be quite flexible in this low-energy range and satisfactory results are obtained with only $N=8$ terms in the basis expansions (2) for partial-waves $L=0$ to $L=15$ to be in complete accord with the available Kohn-Hulthén variational results of Humberston [4] and Brown and Humberston [5] for the S-, P-, D-waves in the Oré gap 6.8 – 10.2 eV. Table 1 shows our total cross section values alongwith those of the Harris-Nesbet variational calculation by Gien [8], and the 21-state close coupling approximation of Mitroy [6]. Our results are in excellent agreement with all these theoretical calculations.

Table 1. The total positronium formation cross section in e⁺-hydrogen collisions in the energy range 6.8 - 10.2 eV.

E(eV)	6.85576	7.65	8.704	9.826
k_i(a.u.)	0.71	0.75	0.80	0.85
Present work	0.0317	0.7507	1.7110	2.6037
Gien [8]	0.0314	0.730	1.663	2.492
Mitroy [6]	0.0313	0.728	1.660	2.49

The total positronium formation cross sections are also found to be in good accord with the recent observed data of the Wayne State group (Zhou *et al* [9]) as is evident from Figure 1. The results of the 33-state calculation of Kernoghan *et al* [7] are shown in this figure. There is satisfactory agreement between these two sets of results.

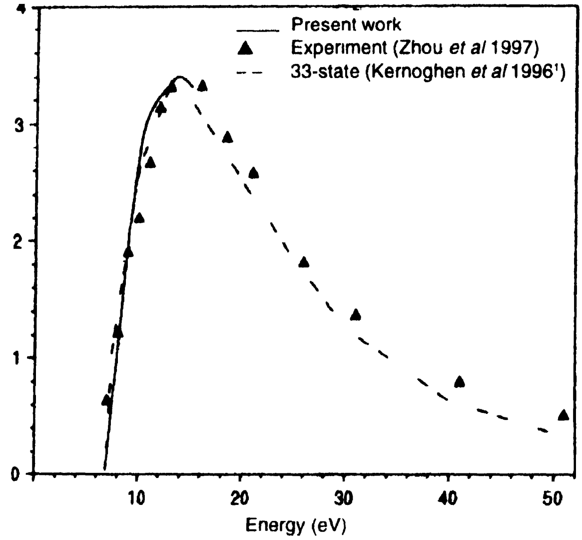

Figure 1. Total cross section for ground-state positronium formation in positron-hydrogen collisions in the energy range 6 8 - 52 0 eV ' Taken from graph

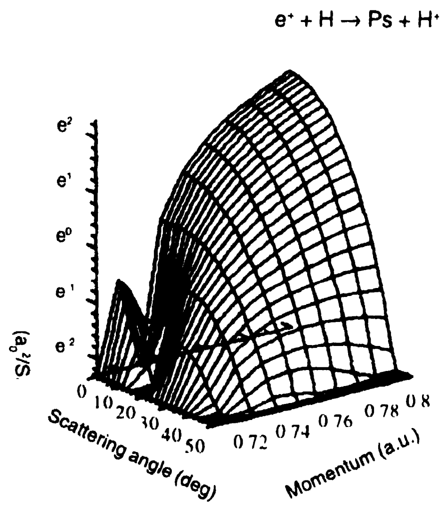

Figure 2. Surface plot of the differential cross section for ground-state positronium formation in positron-hydrogen collisions as a function of energy (6 85576 - 8.704 eV) and scattering angle (0-50 deg)

Our findings indicate the existence of critical angles in positronium formation in positron-hydrogen collisions. These critical angles are found to exist because of the destructive interference between the partial-wave contributions to the scattering amplitude. Surface plots of the positronium formation differential cross section in Figures 2 and 3 display immensely rich structure and the nature of these critical angles.

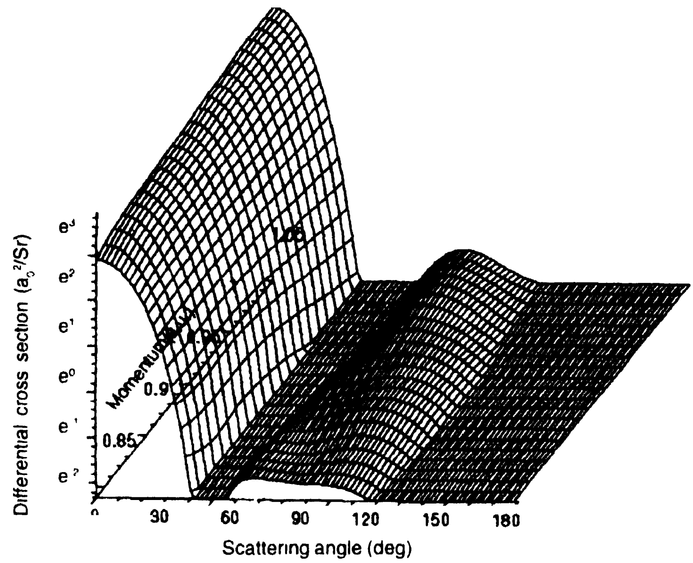

Figure 3. Surface plot of the differential cross section for ground-state positronium formation in positron-H collisions as a function of energy (9 826 - 15 0 eV) and scattering angle (deg)

4. Conclusions

Accurate results are presented for ground-state positronium formation in positron-hydrogen collisions at low-energies using a formulation of the Schwinger's principle for rearrangement collisions. Retaining only $N = 8$ terms of a discrete correlated basis set in both the direct and rearrangement channels with the inverse powers of half-odd integers, it is possible to predict these results which are in satisfactory agreement with the Kohn-Hulthé n and Harris-Nesbet variational calculations [4, 5, 8] and the recent observed data of the Wayne State group [9].

Another interesting feature of this calculation is our finding that it predicts critical angles in positronium formation at incident positron energies from the threshold at 6.8 eV. Surface plots of the differential cross section indicate the nature of these critical angles in great detail.

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